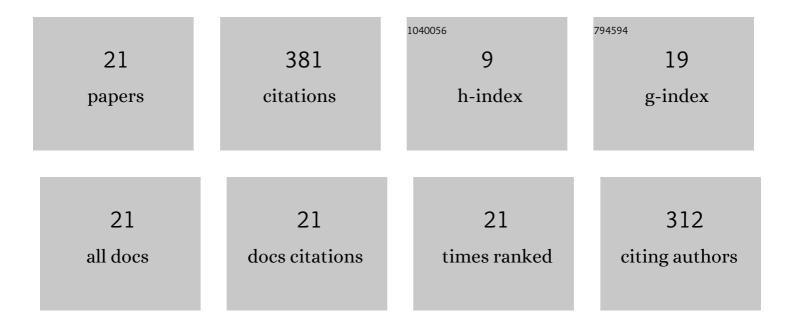
Nayara D Coutinho

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Temperature Dependence of Rate Processes Beyond Arrhenius and Eyring: Activation and Transitivity. Frontiers in Chemistry, 2019, 7, 380.	3.6	69
2	Stereodynamical Origin of Anti-Arrhenius Kinetics: Negative Activation Energy and Roaming for a Four-Atom Reaction. Journal of Physical Chemistry Letters, 2015, 6, 1553-1558.	4.6	63
3	Kinetics of low-temperature transitions and a reaction rate theory from non-equilibrium distributions. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2017, 375, 20160201.	3.4	57
4	Stereodirectional Origin of <i>anti</i> -Arrhenius Kinetics for a Tetraatomic Hydrogen Exchange Reaction: Born–Oppenheimer Molecular Dynamics for OH + HBr. Journal of Physical Chemistry A, 2016, 120, 5408-5417.	2.5	30
5	A novel assessment of the role of the methyl radical and water formation channel in the CH ₃ OH + H reaction. Physical Chemistry Chemical Physics, 2017, 19, 24467-24477.	2.8	22
6	Kinetics of the OH+HCl→H ₂ O+Cl reaction: Rate determining roles of stereodynamics and roaming and of quantum tunneling. Journal of Computational Chemistry, 2018, 39, 2508-2516.	3.3	22
7	Description of the effect of temperature on food systems using the deformed Arrhenius rate law: deviations from linearity in logarithmic plots vs. inverse temperature. Rendiconti Lincei, 2015, 26, 141-149.	2.2	18
8	From statistical thermodynamics to molecular kinetics: the change, the chance and the choice. Rendiconti Lincei, 2018, 29, 787-802.	2.2	18
9	"Transitivity― A Code for Computing Kinetic and Related Parameters in Chemical Transformations and Transport Phenomena. Molecules, 2019, 24, 3478.	3.8	18
10	From the Kinetic Theory of Gases to the Kinetics of Rate Processes: On the Verge of the Thermodynamic and Kinetic Limits. Molecules, 2020, 25, 2098.	3.8	10
11	Topography of the free energy landscape of Claisen–Schmidt condensation: solvent and temperature effects on the rate-controlling step. Physical Chemistry Chemical Physics, 2021, 23, 6738-6745.	2.8	10
12	Description of deviations from Arrhenius behavior in chemical kinetics and materials science. AIP Conference Proceedings, 2016, , .	0.4	9
13	Amino–Imino Tautomerism in the Salt Formation of Albendazole: Hydrobromide and Nitrate Salts. Crystal Growth and Design, 2021, 21, 1122-1135.	3.0	9
14	Temperature dependence of rate constants for the H(D) + CH4 reaction in gas and aqueous phase: deformed Transition-State Theory study including quantum tunneling and diffusion effects. Structural Chemistry, 2020, 31, 609-617.	2.0	8
15	Effect of the Methanol Molecule on the Stabilization of C ₁₈ H ₁₈ O ₄ Crystal: Combined Theoretical and Structural Investigation. Journal of Physical Chemistry A, 2014, 118, 10048-10056.	2.5	5
16	Nucleophilic substitution vs elimination reaction of bisulfide ions with substituted methanes: exploration of chiral selectivity by stereodirectional first-principles dynamics and transition state theory. Journal of Molecular Modeling, 2019, 25, 227.	1.8	5
17	First-Principles Molecular Dynamics and Computed Rate Constants for the Series of OH-HX Reactions (X = H or the Halogens): Non-Arrhenius Kinetics, Stereodynamics and Quantum Tunnel. Lecture Notes in Computer Science, 2018, , 605-623.	1.3	3
18	The \$\$ {mathbf{HI}},varvec{ + },{mathbf{OH}}, o ,{mathbf{H}}_{{mathbf{2}}} {mathbf{O}}, + ,{mathbf{I}} \$\$ HI + OH → H 2 O + I Reaction by First-Principles Molecular Dynamics: Stereodirectional and anti-Arrhenius Kinetics. Lecture Notes in Computer Science, 2017, , 297-313.	1.3	3

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#	Article	IF	CITATIONS
19	The Increase of the Reactivity of Molecular Hydrogen with Hydroxyl Radical from the Gas Phase versus an Aqueous Environment: Quantum Chemistry and Transition State-Theory Calculations. Lecture Notes in Computer Science, 2019, , 450-459.	1.3	1
20	Reply to the â€~Comment on "Topography of the Free Energy Landscape on the Claisen–Schmidt Condensation: Solvent and Temperature Effect in the Rate-Controlling Stepâ€â€™ by N. D. Coutinho, H. G. Machado, V. H. Carvalho-Silva and W. A. da Silva, Phys. Chem. Chem. Phys., 2021, 23, 6738. Physical Chemistry Chemical Physics, 2021, 23, 22202-22206.	2.8	1
21	Rate constants and first-principles trajectories for attack at tetrahedral carbon: Role of molecular orientation on chiral selectivity. AIP Conference Proceedings, 2019, , .	0.4	Ο